4-(1-Cyanoethyl)-1,2,3,4-tetrahydronaphthalene-1-carbonitrile
57964-39-3 | DTXSID2057576

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 22.2

Global applicability domain: Inside

Local applicability domain index: 4.04e-01

Confidence level: 5.51e-01

Nearest Neighbors from the Training Set

Image not found
2-(Thiocyanomethylthio)benzothiazole
Measured: 209
Predicted: 13.0

Image not found
Thiram
Measured: 3.39
Predicted: 3.91

Image not found
Isophorone
Measured: 2.00
Predicted: 3.19

Image not found
Molinate
Measured: 25.7
Predicted: 14.8

Image not found
N,N-Diethylaniline
Measured: 102
Predicted: 12.8